

chain nodes :

7 8 11 12 14 15 17 18 19 20 21 22 24

ring nodes :

1 2 3 4 5 6 25 26 27 28 29 30 31 32 33 34 35 36

chain bonds :

1-20 1-21 2-22 2-24 3-14 4-15 4-17 5-18 5-19 6-33 7-12 7-8  
7-11 26-34

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30  
31-32 31-36 32-33 33-34 34-35 35-36

exact/norm bonds :

1-2 1-6 1-20 1-21 2-3 2-22 2-24 3-4 3-14 4-5 4-15 4-17 5-6  
5-18 5-19 6-33 7-8 26-34 31-32 31-36 32-33 33-34 34-35 35-36

exact bonds :

7-12 7-11

normalized bonds :

25-26 25-30 26-27 27-28 28-29 29-30

isolated ring systems :

containing 1 :

G1:C,H

G2:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 11:CLASS  
12:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS  
21:CLASS

22:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom  
30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 39:Atom

Generic attributes :

8:

Saturation : Unsaturated

Element Count :

Node 8: Limited

N,N1-2

O,O0-1

S,S0-1

# STN Columbus

FULL SCREEN SEARCH COMPLETED - 4290 TO ITERATE

100.0% PROCESSED 4290 ITERATIONS 27 ANSWERS  
SEARCH TIME: 00.00.01

L13 27 SEA SSS FUL L11

=> file caplus

|                      |                  |               |
|----------------------|------------------|---------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST  | 173.54           | 354.02        |

FILE 'CAPLUS' ENTERED AT 12:03:34 ON 19 FEB 2006  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 19 Feb 2006 VOL 144 ISS 9  
FILE LAST UPDATED: 17 Feb 2006 (20060217/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s l13

L14 1 L13

=> d l14 bib abs hitstr

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

## Full Text

AN 2004:650063 CAPLUS

DN 141:174192

TI A preparation of N-containing heterocyclic compounds, useful as 5HT7 antagonists and inverse agonists

IN Bright, Gene Michael; Coffman, Karen J.

PA Pfizer Products Inc., USA

SO PCT Int. Appl., 56 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

|    | PATENT NO.    | KIND | DATE     | APPLICATION NO. | DATE     |
|----|---------------|------|----------|-----------------|----------|
| PI | WO 2004067703 | A2   | 20040812 | WO 2004-IB172   | 20040120 |
|    | WO 2004067703 | A3   | 20041104 |                 |          |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

# STN Columbus

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI  
 CA 2514656 AA 20040812 CA 2004-2514656 20040120  
 EP 1592772 A2 20051109 EP 2004-703447 20040120  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 US 2004229874 A1 20041118 US 2004-766741 20040127  
 PRAI US 2003-444362P P 20030131  
 WO 2004-IB172 W 20040120  
 OS MARPAT 141:174192  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention relates to a prepn. of N-contg. heterocyclic compds. of formula I [wherein: A, B, D, and E are independently CH or N, with at most two of A, B, D, and E being N; Y is a N-contg. heterocycle having 5 to 14 ring atoms and contg. at least one ring nitrogen atom; Z is a deriv. of piperidine, pyrazine, or THF, etc.; R1, R2, and R3 are independently selected from H or (un)substituted alkyl], useful as 5HT7 antagonists and inverse agonists (no biol. data). These compds. are useful as psychotherapeutic agents. For instance, benzoimidazole deriv. II was prepd. via redn. of III (R4 = CHO) and subsequent addn. of benzimidazole to the obtained alc. III (R4 = CH2OH) (example 1).

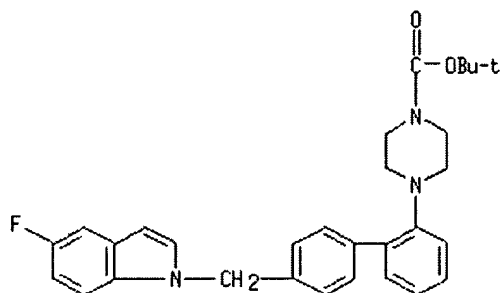
IT 735333-45-6P 735333-47-8P 735333-48-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of N-contg. heterocyclic compds. useful as 5HT7 antagonists and inverse agonists)

RN 735333-45-6 CAPLUS

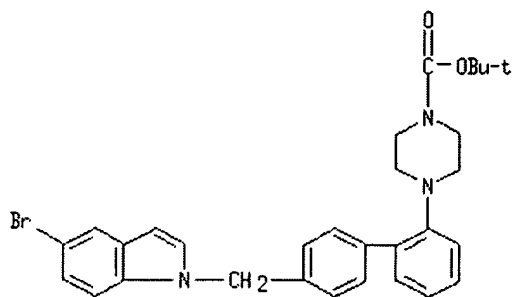
CN 1-Piperazinecarboxylic acid, 4-[4'-[(5-fluoro-1H-indol-1-yl)methyl][1,1'-biphenyl]-2-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 735333-47-8 CAPLUS

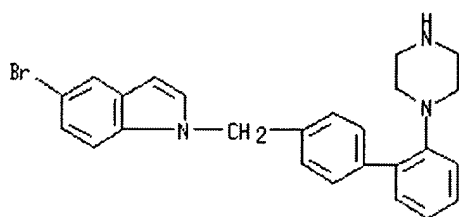
CN 1-Piperazinecarboxylic acid, 4-[4'-[(5-bromo-1H-indol-1-yl)methyl][1,1'-biphenyl]-2-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

STN Columbus



RN 735333-48-9 CAPLUS

CN 1H-Indole, 5-bromo-1-[[2'-(1-piperazinyl)[1,1'-biphenyl]-4-yl]methyl]-  
(9CI) (CA INDEX NAME)



IT 735333-38-7P 735333-39-8P 735333-40-1P

735333-41-2P 735333-42-3P 735333-46-7P

735333-49-0P 735333-52-5P 735333-54-7P

735333-56-9P 735333-58-1P 735333-60-5P

735333-77-4P 735333-78-5P 735333-79-6P

735333-80-9P 735333-81-0P 735333-82-1P

735333-83-2P 735333-84-3P 735333-85-4P

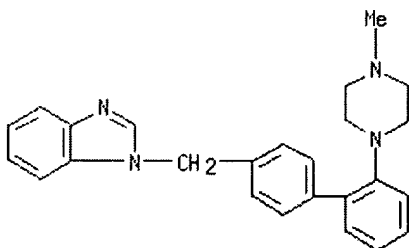
735333-86-5P 735333-87-6P 735333-88-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(prepn. of N-contg. heterocyclic compds. useful as 5HT7 antagonists and  
inverse agonists)

RN 735333-38-7 CAPLUS

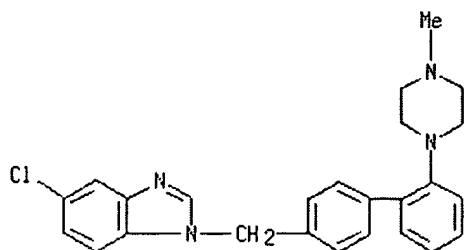
CN 1H-Benzimidazole, 1-[[2'-(4-methyl-1-piperazinyl)[1,1'-biphenyl]-4-  
yl]methyl]- (9CI) (CA INDEX NAME)



RN 735333-39-8 CAPLUS

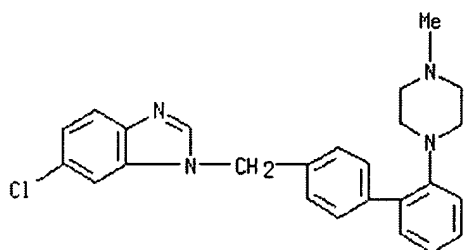
CN 1H-Benzimidazole, 5-chloro-1-[[2'-(4-methyl-1-piperazinyl)[1,1'-biphenyl]-  
4-yl]methyl]- (9CI) (CA INDEX NAME)

# STN Columbus



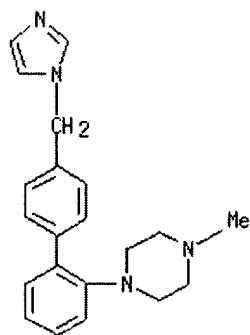
RN 735333-40-1 CAPLUS

CN 1H-Benzimidazole, 6-chloro-1-[[2'-(4-methyl-1-piperazinyl) [1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



RN 735333-41-2 CAPLUS

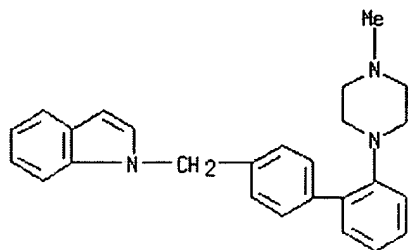
CN Piperazine, 1-[4'-(1H-imidazol-1-ylmethyl) [1,1'-biphenyl]-2-yl]-4-methyl- (9CI) (CA INDEX NAME)



RN 735333-42-3 CAPLUS

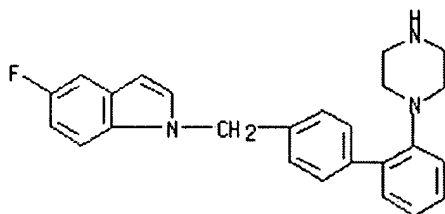
CN 1H-Indole, 1-[[2'-(4-methyl-1-piperazinyl) [1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)

STN Columbus



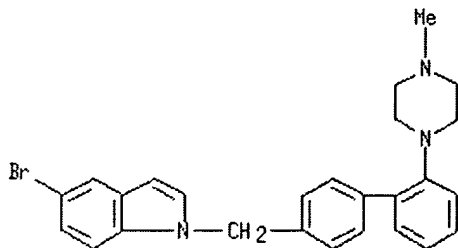
RN 735333-46-7 CAPLUS

CN 1H-Indole, 5-fluoro-1-[[2'-(1-piperazinyl)[1,1'-biphenyl]-4-yl]methyl]-  
(9CI) (CA INDEX NAME)



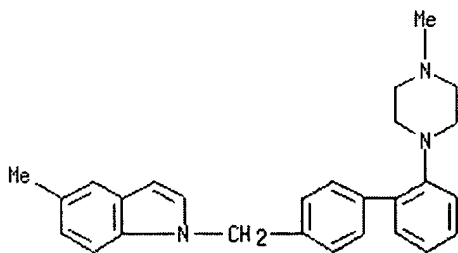
RN 735333-49-0 CAPLUS

CN 1H-Indole, 5-bromo-1-[[2'-(4-methyl-1-piperazinyl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



RN 735333-52-5 CAPLUS

CN 1H-Indole, 5-methyl-1-[[2'-(4-methyl-1-piperazinyl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)

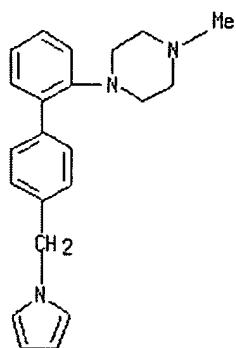


RN 735333-54-7 CAPLUS

CN Piperazine, 1-methyl-4-[4'-(1H-pyrrol-1-ylmethyl)[1,1'-biphenyl]-2-yl]-

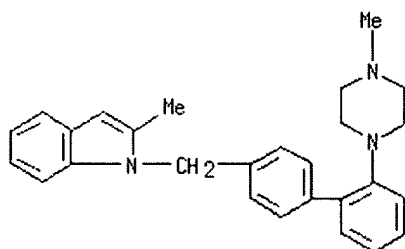
# STN Columbus

(9CI) (CA INDEX NAME)



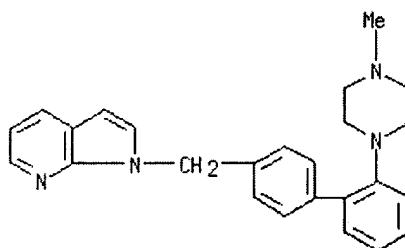
RN 735333-56-9 CAPLUS

CN 1H-Indole, 2-methyl-1-[[2'-(4-methyl-1-piperazinyl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



RN 735333-58-1 CAPLUS

CN 1H-Pyrrolo[2,3-b]pyridine, 1-[[2'-(4-methyl-1-piperazinyl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)

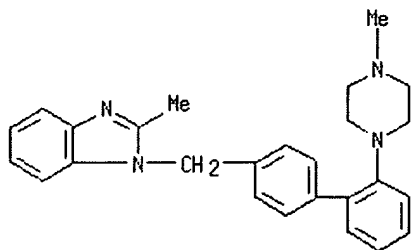


RN 735333-60-5 CAPLUS

CN 1H-Benzimidazole, 2-methyl-1-[[2'-(4-methyl-1-piperazinyl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)

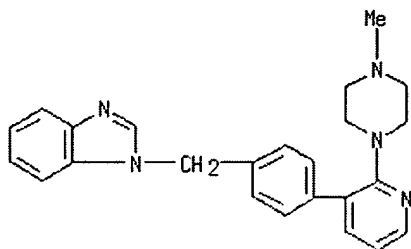


STN Columbus



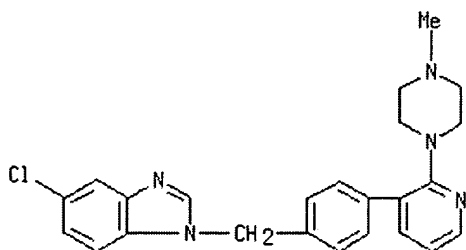
RN 735333-77-4 CAPLUS

CN 1H-Benzimidazole, 1-[[4-[2-(4-methyl-1-piperazinyl)-3-pyridinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



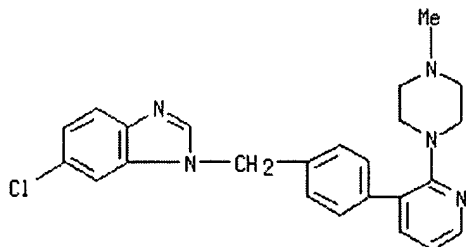
RN 735333-78-5 CAPLUS

CN 1H-Benzimidazole, 5-chloro-1-[[4-[2-(4-methyl-1-piperazinyl)-3-pyridinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 735333-79-6 CAPLUS

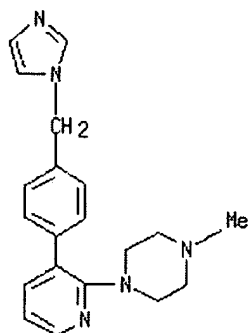
CN 1H-Benzimidazole, 6-chloro-1-[[4-[2-(4-methyl-1-piperazinyl)-3-pyridinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 735333-80-9 CAPLUS

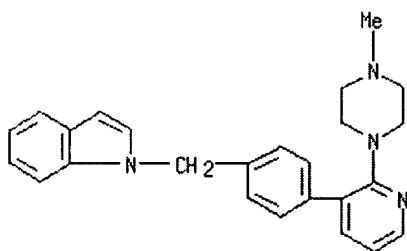
# STN Columbus

CN Piperazine, 1-[3-[4-(1H-imidazol-1-ylmethyl)phenyl]-2-pyridinyl]-4-methyl-  
(9CI) (CA INDEX NAME)



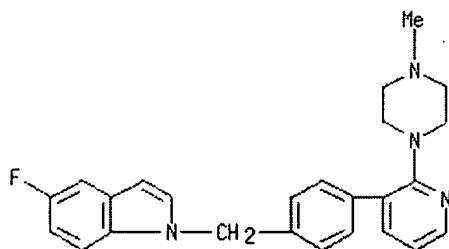
RN 735333-81-0 CAPLUS

CN 1H-Indole, 1-[[4-[2-(4-methyl-1-piperazinyl)-3-pyridinyl]phenyl]methyl]-  
(9CI) (CA INDEX NAME)



RN 735333-82-1 CAPLUS

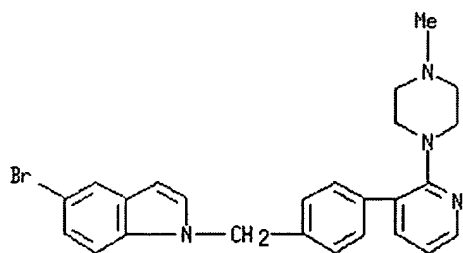
CN 1H-Indole, 5-fluoro-1-[[4-[2-(4-methyl-1-piperazinyl)-3-pyridinyl]phenyl]methyl]-  
(9CI) (CA INDEX NAME)



RN 735333-83-2 CAPLUS

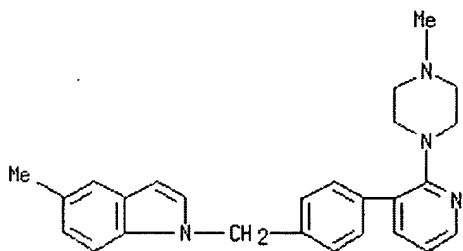
CN 1H-Indole, 5-bromo-1-[[4-[2-(4-methyl-1-piperazinyl)-3-pyridinyl]phenyl]methyl]-  
(9CI) (CA INDEX NAME)

STN Columbus



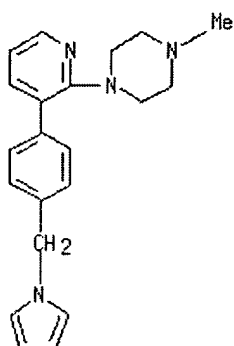
RN 735333-84-3 CAPLUS

CN 1H-Indole, 5-methyl-1-[[4-[2-(4-methyl-1-piperazinyl)-3-pyridinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 735333-85-4 CAPLUS

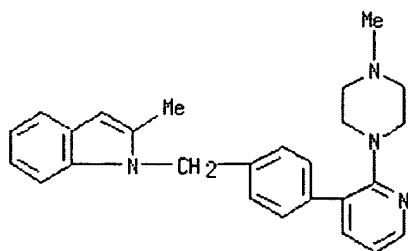
CN Piperazine, 1-methyl-4-[3-[4-(1H-pyrrol-1-ylmethyl)phenyl]-2-pyridinyl]- (9CI) (CA INDEX NAME)



RN 735333-86-5 CAPLUS

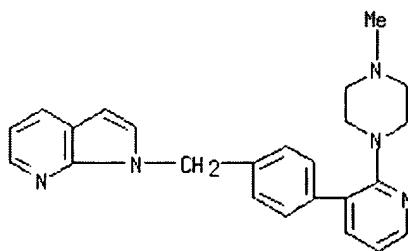
CN 1H-Indole, 2-methyl-1-[[4-[2-(4-methyl-1-piperazinyl)-3-pyridinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

## STN Columbus



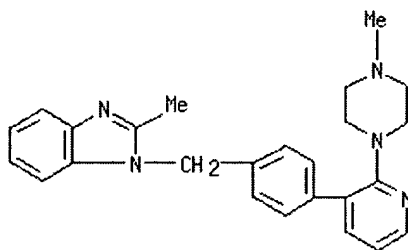
RN 735333-87-6 CAPLUS

CN 1H-Pyrrolo[2,3-b]pyridine, 1-[[4-[2-(4-methyl-1-piperazinyl)-3-pyridinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 735333-88-7 CAPLUS

CN 1H-Benzimidazole, 2-methyl-1-[[4-[2-(4-methyl-1-piperazinyl)-3-pyridinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



=&gt; file caold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

5.57

359.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.75

-0.75

FILE 'CAOLD' ENTERED AT 12:04:25 ON 19 FEB 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

## STN Columbus

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

```
=> s l13
L15      0 L13

=>
```